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ABSTRACT

During the period of the grant an interrelated set of studies were performed in the general domain of control over quantum dynamics phenomena. A prime focus was on establishing the basic principles of quantum control and their experimental implications. The overall research is summarized below.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

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Received		<u>Paper</u>
09/14/2011	10.00	A. Donovan, V. Beltrani, H. Rabitz. Quantum control by means of Hamiltonian structure manipulation, Physical Chemistry Chemical Physics, (02 2011): 7348. doi: 10.1039/c0cp02234a
09/14/2011	14.00	Ariana Rondi, Denis Kiselev, Sarah Machado, Jérôme Extermann, Stefan Weber, Luigi Bonacina, Jean-Pierre Wolf, Jonathan Roslund, Matthias Roth, Herschel Rabitz. Discriminating Biomolecules with Coherent Control Strategies, CHIMIA, (05 2011): 346. doi: 10.2533/chimia.2011.346
09/14/2011	13.00	Jonathan Roslund, Matthias Roth, Laurent Guyon, Ve?ronique Boutou, Francois Courvoisier, Jean-Pierre Wolf, Herschel Rabitz. Resolution of strongly competitive product channels with optimal dynamic discrimination: Application to flavins, The Journal of Chemical Physics, (01 2011): 34511. doi: 10.1063/1.3518751
09/14/2011	12.00	A. Shabani, M. Mohseni, S. Lloyd, R. Kosut, H. Rabitz. Efficient estimation of spare many-body quantum Hamiltonians, Physical Review A, (7 2011): 1. doi: 10.1103/PhysRevA.84.012107
10/05/2010	7.00	Renan Cabrera and Herschel Rabitz Calculation of the unitary part of the Bures measure for N-level quantum systems
		Journal of Physics A: Mathematical and Theoretical, (10 2009): . doi:
10/05/2010	8.00	Roberto Rey-de-Castro, Herschel Rabitz . Laboratory implementation of quantum-control-mechanism identification through Hamiltonian encoding and observable decoding
		, Physical Review A, (06 2010): . doi:
10/05/2010	9.00	Alexander Pechen, Constantin Brif, Rebing Wu, Raj Chakraharti, and Herschel Rabitz . General unifying features of controlled quantum phenomena
		Physical Review A, (09 2010): . doi:
10/05/2010	5.00	Matthew D Grace, Jason Dominy, Robert L Kosut, Constantin Brif and Herschel Rabitz. Environment-invariant measure of distance between evolutions of an open quantum system, New Journal of Physics, (01 2010): . doi:
10/05/2010	6.00	Constantin Brif, Raj Chakrabarti, Herschel Rabitz. Controlofquantum phenomena: past, presentand future, New Journal of Physics, (07 2010): . doi:
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09/14/2011	11.00 Michael Klein, Vincent Beltrani, Herschel Rabitz. Features of quantum control in the sudd (07 2010)	len regime,
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During the period of the grant an interrelated set of studies were performed in the general domain of control over quantum dynamics phenomena. A prime focus was on establishing the basic principles of quantum control and their experimental implications. The overall research is summarized below.

1. Calculation of the unitary part of the Bures measure for n□level quantum systems

Renan Cabrera and Herschel Rabitz - J. Chem. Phys., 42/445302(2009).

We use the canonical coset parameterization and provide a formula with the unitary part of the Bures measure for nondegenerate systems in terms of the product of even Euclidean balls. This formula is shown to be consistent with the sampling of random states through the generation of random unitary matrices.

2. Exploring the capabilities of quantum optimal dynamic discrimination

Vincent Beltrani, Pritha Ghosh, and Herschel Rabitz - J. Chem. Phys., 130, 164112 (2009).

Optimal dynamic discrimination uses closed-loop learning control techniques to discriminate between similar quantum systems. ODD achieves discrimination by employing a shaped control <code>2laser2</code> pulse to simultaneously exploit the unique quantum dynamics particular to each system, even when they are quite similar. In this work, ODD is viewed in the context of multiobjective optimization, where the competing objectives are the degree of similarity of the quantum systems and the level of controlled discrimination that can be achieved. To facilitate this study, the D-MORPH gradient algorithm is extended to handle multiple quantum systems and multiple objectives. This work explores the trade-off between laser resources <code>2e.g.</code>, the length of the pulse, fluence, etc. and ODD's ability to discriminate between similar systems. A mechanism analysis is performed to identify the dominant pathways utilized to achieve discrimination between similar systems.

3. Quantum control implemented as combinatorial optimization

Strohecker T, Rabitz H. - J. Comput Chem 31:151-153 (2010).

Optimal control theory provides a general means for designing controls to manipulate quantum phenomena. Traditional implementation requires solving coupled nonlinear equations to obtain the optimal control solution, whereas this work introduces a combinatorial quantum control (CQC) algorithm to avoid this complexity. The CQC technique uses a predetermined toolkit of small time step propagators in conjunction with combinatorial optimization to identify a proper sequence for the toolkit members. Results indicate that the CQC technique exhibits invariance of search effort to the number of system states and very favorable scaling upon comparison to a standard gradient algorithm, taking into consideration that

Principal Investigator: Herschel Rabitz Time Period Covered: 9/1/2009-8/31/2012

CQC is easily parallelizable.

4. Laboratory implementation of quantum control mechanism identification through Hamiltonian-encoding and observable decoding

Rey-de-Castro and H. Rabitz, Phys. Rev. A, 81, 063422 (2010).

We report on the laboratory implementation of quantum-control-mechanism identification through Hamiltonian encoding and observable decoding (HE-OD). Over a sequence of experiments, HE-OD introduces a special encoded signature into the components of a previously determined control field expressed in a chosen representation. The outcome appears as a modulated signal in the controlled system observable. Decoding the modulated signal identifies the hierarchy of correlations between components of the control field in a particular representation. In cases where the initial quantum state and observable operator are fully known, then HE-OD can also identify the transition amplitudes of the various Dyson expansion orders contributing to the controlled dynamics. The basic principles of HE-OD are illustrated for second harmonic generation when the components of the field representation are simply taken as the pixels in the pulse shaper. The outcome of HE-OD agrees well with simulations, verifying the concept.

5. Unified analysis of terminal-time control in classical and quantum systems A. Pechen and H. Rabitz, EPL, 91, 10006 (2010).

Many phenomena in physics, chemistry, and biology involve seeking an optimal control to maximize an objective for a classical or quantum system which is open and interacting with its environment. The complexity of finding an optimal control for maximizing an objective is strongly affected by the possible existence of sub-optimal maxima. Within a unified framework under specified conditions, control objectives for maximizing at a terminal-time physical observables of open classical and quantum systems are shown to be inherently free of sub-optimal maxima. This attractive feature is of central importance for enabling the discovery of controls in a seamless fashion in a wide range of phenomena transcending the quantum and classical regimes.

6. General unifying features of controlled quantum phenomena 2

A. Pechen, C. Brif, R. Wu, R. Chakrabarti, H. Rabitz, Phys. Rev. A., 82, 030101 (2010).

Principal Investigator: Herschel Rabitz Time Period Covered: 9/1/2009-8/31/2012

Many proposals have been put forth for controlling quantum phenomena, including open-loop, adaptive feedback, and real-time feedback control. Each of these approaches has been viewed as operationally, and even physically, distinct from the others. This work shows that all such scenarios inherently share the same fundamental control features residing in the topology of the landscape relating the target physical observable to the applied controls. This unified foundation may provide a basis for development of hybrid control schemes that would combine the advantages of the existing approaches to achieve the best overall performance.

7. Features of quantum control in the sudden regime 2

M. Klein, V. Beltrani, H. Rabitz, Chem. Phys. Lett., 499, 161 (2010).

Although quantum dynamics in the sudden regime is generally not fully controllable, the simple dependence of the observable yield on the applied field enables efficient searches for a control and also admits generally many solutions. This flexibility allows for simultaneous optimization of ancillary objectives including the minimization of competing pathways throughout the control period. These features are illustrated with simple models and simulations.

8. Environment-invariant measure of distance between evolutions of an open quantum system 2

M. Grace, J. Dominy, R. Kosut, C. Brif and H. Rabitz, New J. of Phys., 12, 015001 (2010).

In this work we analyze the quantum controllability of rotational motion under the influence of an external laser field coupled through a permanent dipole moment. The analysis takes into consideration up to three polarization fields, but we also discuss the consequences for working with fewer polarized fields.

9. The canonical coset decomposition of unitary matrices through Householder transformations 2

R. Cabrera, T. Strohecker and H. Rabitz, J. Math. Phys., 51, 082101 (2010).

This paper reveals the relation between the canonical coset decomposition of unitary matrices and the corresponding decomposition via Householder reflections. These results can be used to parametrize unitary matrices via Householder reflections.

10. Quantum control by means of Hamiltonian structure manipulation 2

A. Donovan, V. Beltrani and H. Rabitz, Phys. Chem. Chem. Phys., 13, 7348 (2011).

A traditional quantum optimal control experiment begins with a specific physical system and seeks an optimal time-dependent field to steer the evolution towards a target observable value. In a more general framework, the Hamiltonian structure may

Principal Investigator: Herschel Rabitz Time Period Covered: 9/1/2009-8/31/2012

also be manipulated when the material or molecular 'stockroom' is accessible as a part of the controls. The current work takes a step in this direction by considering the converse of the normal perspective to now start with a specific fixed field and employ the system's time-independent Hamiltonian structure as the control to identify an optimal form. The Hamiltonian structure control variables are taken as the system energies and transition dipole matrix elements. An analysis is presented of the Hamiltonian structure control landscape, defined by the observable as a function of the Hamiltonian structure. A proof of system controllability is provided, showing the existence of a Hamiltonian structure that yields an arbitrary unitary transformation when working with virtually any field. The landscape analysis shows that there are no suboptimal traps (i.e., local extrema) for controllable quantum systems when unconstrained structural controls are utilized to optimize a state-to-state transition probability. This analysis is corroborated by numerical simulations on model multilevel systems. The search effort to reach the top of the Hamiltonian structure landscape is found to be nearly invariant to system dimension. A control mechanism analysis is performed, showing a wide variety of behavior for different systems at the top of the Hamiltonian structure landscape. It is also shown that reducing the number of available Hamiltonian structure controls, thus constraining the system, does not always prevent reaching the landscape top. The results from this work lay a foundation for considering the laboratory implementation of optimal Hamiltonian structure manipulation for seeking the best control performance, especially with limited electromagnetic resources.

11. Hamiltonian reduction of quantum systems controlled by pulses 2

Q. Xu, Y. Wang F. Shuang, H. Rabitz, Chin. J. Chem. Phys., 24, 378 (2011).

We explore Hamiltonian reduction in pulse-controlled finite-dimensional quantum systems with near-degenerate eigenstates. A quantum system with a non-degenerate ground state and several near-degenerate excited states is controlled by a short pulse, and the objective is to maximize the collective population on all excited states when we treat all of them as one level. Two cases of the systems are shown to be equivalent to effective two-level systems. When the pulse is weak, simple relations between the original systems and the reduced systems are obtained. When the pulse is strong, these relations are still available for pulses with only one frequency under the first-order approximation.

K. Moore, A. Pechen, X-J Feng, J. Dominy, V. Beltrani and H. Rabitz, Phys. Chem. Chem. Phys., DOI: 10.1039/C1CP20353C (2011).

Identifying optimal conditions for chemical and material synthesis as well as optimizing the properties of the products is often much easier than simple reasoning would predict. The potential search space is infinite in principle and enormous in practice,

Principal Investigator: Herschel Rabitz Time Period Covered: 9/1/2009-8/31/2012

yet optimal molecules, materials, and synthesis conditions for many objectives can often be found by performing a reasonable number of distinct experiments. Considering the goal of chemical synthesis or property identification as optimal control problems provides insight into this good fortune. Both of these goals may be described by a fitness function J that depends on a suitable set of variables (e.g., reactant concentrations, components of a material, processing conditions, etc.). The relationship between J and the variables specifies the fitness landscape for the target objective. Upon making simple physical assumptions, this work demonstrates that the fitness landscape for chemical optimization contains no local sub-optimal maxima that may hinder attainment of the absolute best value of J. This feature provides a basis to explain the many reported efficient optimizations of synthesis conditions and molecular or material properties. We refer to this development as OptiChem theory. The predicted characteristics of chemical fitness landscapes are assessed through a broad examination of the recent literature, which shows ample evidence of trap-free landscapes for many objectives. The fundamental and practical implications of OptiChem theory for chemistry are discussed.

14. Optimal dynamic detection enhances sensitivity of explosives detection 2

S. McGrane, M. Greenfield, J. Scharff, D. Moore, J. Roslund and H. Rabitz, Laser Focus World, 2 (2011).

Principal Investigator: Herschel Rabitz Time Period Covered: 9/1/2009-8/31/2012

A new Optimal Dynamic Detection (ODD) technology based on shaped laser pulses simultaneously enhances explosive signature sensitivity while reducing the influence of noise and the signals from background interference in the field.

15. A general formulation of monotonically convergent algorithms in the control of quantum dynamics beyond the linear dipole interaction 2

T.-S. Ho, H. Rabitz and S.-I. Chu, Comp. Phys. Comm., 182, 14 (2011).

This paper presents a general method to formulate monotonically convergent algorithms for identifying optimal control fields to manipulate quantum dynamics phenomena beyond the linear dipole interaction. The method, facilitated by a field-dependent dipole moment operator, is based on an integral equation of the first kind arising from the Heisenberg equation of motion for tracking a time-dependent, dynamical invariant observable associated with a reference control field.

16. Multiobjective adaptive feedback control of two-photon absorption coupled with propagation 2

F. Laforge, J. Roslund, O. Shir and H. Rabitz, Phys. Rev. A, 84, 013401 (2011).

This work uses shaped femtosecond laser pulses to control the two-photon absorption (TPA) of coumarin 153 in a dispersive toluene medium. The dispersive medium reshapes the pulse along the optical path, and management of this effect is used to achieve spatial localization of TPA. Other control objectives were successfully implemented, including dual localization and high resolution local optimization of TPA. The solutions to these objectives were explored by means of evolutionary single-and multi-objective algorithms within a laboratory feedback loop.

17. Attaining persistent field-free control of open and closed quantum systems 2

E. Anson, V. Beltrani and H. Rabitz, J. Chem. Phys. 134, 124110 (2011).

Persistent quantum control (PQC) aims to maintain an observable objective value over a period of time following the action of an applied field. This paper assesses the feasibility of achieving PQC for arbitrary finite-level systems and observables. The analysis is carried out independent of the particular method used for state preparation. The PQC behavior is optimized over the set of physically accessible prepared states for both open and closed systems. The quality of observable value persistence in the post-control period was found to vary with the required duration of persistence, the system temperature, the chosen observable operator, and the energy levels of the system. The alignment of a rigid diatomic rotor is studied as a model system. The theoretical estimates of PQC behavior are encouraging and suggest feasible exploration in the laboratory using currently available technology.

Principal Investigator: Herschel Rabitz Time Period Covered: 9/1/2009-8/31/2012

18. Exploring the top and bottom of the quantum control landscape 2

V. Beltrani, J. Dominy, TS Ho, H. Rabitz, J. Chem. Phys., 134, 194106 (2011).

A controlled quantum system possesses a search landscape defined by the target physical objective as a function of the controls. This paper focuses on the landscape for the transition probability $Pi \rightarrow f$ between the states of a finite level quantum system. Traditionally, the controls are applied fields; here, we extend the notion of control to also include the Hamiltonian structure, in the form of time independent matrix elements. Level sets of controls that produce the same transition probability value are shown to exist at the bottom $Pi \rightarrow f = 0.0$ and top $Pi \rightarrow f = 1.0$ of the landscape with the field and/or Hamiltonian structure as controls. We present an algorithm to continuously explore these level sets starting from an initial point residing at either extreme value of $Pi \rightarrow f$. The technique can also identify control solutions that exhibit the desirable properties of (a) robustness at the top and (b) the ability to rapidly rise towards an optimal control from the bottom. Numerical simulations are presented to illustrate the varied control behavior at the top and bottom of the landscape for several simple model systems.

19. Bounds on the curvature at the top and bottom of the transition probability landscape [2]

V. Beltrani, J. Dominy, T.-S. Ho and H. Rabitz, J. Phys. B, 44, 154009 (2011).

The transition probability between the states of a controlled quantum system is a basic physical observable, and the associated control landscape is specified by the transition probability as a function of the applied field. An initial control likely will produce a transition probability near the bottom of the landscape, while the final goal is to find a field that results in a high transition probability value at the top. For controls producing either of the latter extreme landscape values, the Hessian of the transition probability with respect to the control field characterizes the curvature of the landscape and the ease of leaving either limit. Prior work showed that the Hessian spectrum possesses an upper bound on the number of non-zero eigenvalues as well as an infinite number of zero eigenvalues. The associated eigenfunctions accordingly specify the coordinated control field changes that either maximally or minimally influence the transition probability. We show in this paper that there exists a lower bound on the number of non-zero Hessian eigenvalues at either the top or bottom of the landscape. In particular, there is at least one non-zero eigenvalue at the top and generally one at the bottom. Under special circumstances, the Hessian may be identically zero at the bottom (i.e. it possesses no non-zero eigenvalues). These results dictate the curvature of the top and bottom of the landscape, which has important physical significance for seeking optimal control fields. At the top, a field that produces a single non-zero Hessian eigenvalue of small magnitude will generally exhibit a high degree of robustness to field

Principal Investigator: Herschel Rabitz Time Period Covered: 9/1/2009-8/31/2012

noise. In contrast, at the bottom, working with a field producing the maximum number of non-zero eigenvalues will generally assure the most rapid climb towards a high transition probability.

20. Fidelity between unitary operators and the generation of robust gates against off-resonance perturbation R. Cabrera, O. Shir, R. Wu and H. Rabitz, J. Phys A, 44, 095302 (2011).

We perform a functional expansion of the fidelity between two unitary matrices in order to find necessary conditions for the robust implementation of a target gate. Comparison of these conditions with those obtained from the Magnus expansion and Dyson series shows that they are equivalent in the first order. By exploiting techniques from *robust design optimization*, we account for issues of experimental feasibility by introducing an additional criterion to the search for control pulses. This search is accomplished by exploring the competition between the multiple objectives in the implementation of the NOT gate by means of evolutionary multi-objective optimization.

21. Control of Quantum Phenomena 2

C. Brif, R. Chakrabati, H. Rabitz, in Advances in Chemical Physics, Volume 148 (eds S. A. Rice and A. R. Dinner), John Wiley & Sons, Inc., Hoboken, NJ, USA. DOI: 10.1002/9781118158715. ch1

This work presented a thorough review of the recent quantum control literature. A particular emphasis was placed on the theoretical foundations o the field and the body of closed loop experiments.

22. Quantum control experiments as a testbed for evolutionary multi-objective algorithms

Ofer M. Shir, Jonathan Roslund, Zaki Leghtas, Herschel Rabitz Genet Program Evolvable Mach 13:445–491 DOI 10.1007/s10710-012-9164-7 (2012)

Experimental multi-objective Quantum Control is an emerging topic within the broad physics and chemistry applications domain of controlling quantum phenomena. This realm offers cutting edge ultrafast laser laboratory applications, which pose multiple objectives, noise, and possibly constraints on the high-dimensional search. In this study we introduce the topic of multi-observable quantum control (MOQC), and consider specific systems to be Pareto optimized subject to uncertainty, either *experimentally* or by means of simulated systems. The latter include a family of mathematical test-functions with a practical link to MOQC experiments, which are introduced here for the first time. We investigate the behavior of the multi-objective version of the covariance matrix adaptation evolution strategy (MO-CMA-ES) and assess its performance on computer simulations as well as on laboratory closed-loop experiments. Overall, we propose a comprehensive study on *experimental*

Principal Investigator: Herschel Rabitz Time Period Covered: 9/1/2009-8/31/2012

evolutionary Pareto optimization in high-dimensional continuous domains, draw some *practical* conclusions concerning the impact of fitness disturbance on algorithmic behavior, and raise several *theoretical* issues in the broad evolutionary multi-objective context

23. Exploiting time-independent Hamiltonian structure as controls for manipulating quantum dynamics.

Beltrani V, Rabitz H - J Chem Phys. 137(9):094109. doi: 10.1063/1.4743954. (2012)

The opportunities offered by utilizing time-independent Hamiltonian structure as controls are explored for manipulating quantum dynamics. Two scenarios are investigated using different manifestations of Hamiltonian structure to illustrate the generality of the concept. In scenario I, optimally shaped electrostatic potentials are generated to flexibly control electron scattering in a two-dimensional subsurface plane of a semiconductor. A simulation is performed showing the utility of optimally setting the individual voltages applied to a multi-pixel surface gate array in order to produce a spatially inhomogeneous potential within the subsurface scattering plane. The coherent constructive and destructive electron wave interferences are manipulated by optimally adjusting the potential shapes to alter the scattering patterns. In scenario II, molecular vibrational wave packets are controlled by means of optimally selecting the Hamiltonian structure in cooperation with an applied field. As an illustration of the concept, a collection (i.e., a level set) of dipole functions is identified where each member serves with the same applied electric field to produce the desired final transition probability. The level set algorithm additionally found Hamiltonian structure controls exhibiting desirable physical properties. The prospects of utilizing the applied field and Hamiltonian structure simultaneously as controls is also explored. The control scenarios I and II indicate the gains offered by algorithmically guided molecular or material discovery for manipulating quantum dynamics phenomenon.

24. Dynamic Homotopy and Landscape Dynamical Set Topology in Quantum Control

Jason Dominy, Herschel Rabitz. - J. Math Physics 53,8 (2012)

We examine the topology of the subset of controls taking a given initial state to a given final state in quantum control, where "state" may mean a pure state $|\psi|$, an ensemble density matrix ρ , or a unitary propagator U(0, T). The analysis consists in showing that the endpoint map acting on control space is a Hurewicz fibration for a large class of affine control systems with vector controls. Exploiting the resulting fibration sequence and the long exact sequence of basepoint-preserving homotopy classes of maps, we show that the indicated subset of controls is homotopy equivalent to the loopspace of the state manifold. This not only allows us to understand the connectedness of "dynamical sets" realized as preimages of subsets of the state space through this endpoint map, but also provides a wealth of additional topological information about such subsets of

Principal Investigator: Herschel Rabitz

Time Period Covered: 9/1/2009-8/31/2012

control space.